

Dynamic symmetry breaking in a 2D electron gas with a spectral node

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We study a 2D electron gas with a spectral node and a random gap in a vicinity of the node. After identifying the fundamental dynamic symmetries of this system, the spontaneous breaking of the latter by a Grassmann field is studied within a nonlinear sigma model approach. This allows us to reduce the average two-particle Green's function to a diffusion propagator with a random diffusion coefficient. The latter has non-degenerate saddle points and is treated by the conventional self-consistent Born approximation. This leads to a renormalized chemical potential and diffusion coefficient, where the DC conductivity increases linearly with the density of quasiparticles.

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The prototype of a 2D electron gas with spectral nodes is graphene, where two symmetric electronic bands, created by the underlying honeycomb lattice structure, touch each other at two different points in the Brillouin zone [1–4]. The surface states of the recently discovered topological insulators is another example for spectral nodes [5]. It is a remarkable experimental fact that the two-dimensional electron gas in graphene is always in a metallic state, regardless of its Fermi energy, provided that the sublattice symmetry of the honeycomb lattice is unbroken. This is particularly surprising from the theoretical point of view, since the electron gas should be in a localized state, at least away from the node (Dirac point) [6]. At the Dirac point, however, the underlying Hamiltonian has an extra particle-hole symmetry, depending on the type of disorder though, which may be responsible for metallic (diffusive) behavior. The experimentally observed metallic state at and away from the node indicates that the diffusive behavior may not depend on this extra symmetry. We shall discuss in the following that a dynamical symmetry exists which is responsible, regardless of the chemical potential, for a diffusive behavior.

Many characteristic properties of a quantum system, in particular the spectral and large scale properties, are determined by symmetry properties of the underlying Hamiltonian. However, for the dynamics of a quantum system additional symmetries play a role, because the dynamics is not only controlled by the real spectrum but also on the complex plane by the advanced and the retarded Green's function $G(\pm i\epsilon) = (H \pm i\epsilon)^{-1}$, which are related by Hermitian conjugation: $G(-i\epsilon) = G^\dagger(i\epsilon)$. An example is the transition probability [7]

$$P_{\mathbf{r},\mathbf{r}'}(i\epsilon) = K_{\mathbf{r},\mathbf{r}'}(i\epsilon) / \sum_{\mathbf{r}} K_{\mathbf{r},\mathbf{r}'}(i\epsilon) \quad (1)$$

with

$$K_{\mathbf{r},\mathbf{r}'}(i\epsilon) = \langle G_{\mathbf{r},\mathbf{r}'}(i\epsilon) G_{\mathbf{r}',\mathbf{r}}(-i\epsilon) \rangle_v. \quad (2)$$

The average is here with respect to a random variable (e.g. random potential or a random gap) in the Hamiltonian H . Randomness is necessary to provide scattering that breaks translational invariance. It is convenient to combine the two Green's functions in the extended Green's function

$$\hat{G}(i\epsilon) = \begin{pmatrix} (H + i\epsilon)^{-1} & 0 \\ 0 & (H - i\epsilon)^{-1} \end{pmatrix} \quad (3)$$

such that with $\hat{H} = \text{diag}(H, H)$ we have $\hat{G}(i\epsilon) = (\hat{H} + i\epsilon\hat{\sigma}_3)^{-1}$. Then there is an orthogonal or unitary symmetry which rotates the two-dimensional space that is spanned by the two Hamiltonians. It has been found long time ago that the symmetry breaking due to ϵ can cause spontaneous symmetry breaking in the limit $\epsilon \rightarrow 0$. The corresponding massless mode leads to a diffusive behavior [8, 9].

The definition of (3) was also used as the starting point for Dirac fermions with random mass by Bocquet et al. [10]. Employing a supersymmetric representation, where $\hat{G}(i\epsilon)$ is applied to a Bose and to a Fermi field, the gradient expansion of the effective field theory produces an orthosymplectic nonlinear sigma model in this case. Unfortunately, the analysis of the latter is quite involved and the transport properties cannot be easily extracted.

Prior to the work by Bocquet et al., an alternative approach was suggested by the present author [11] using explicitly the fact that the Dirac Hamiltonian $H = i\sigma_k \partial_k + m\sigma_3$ (σ_j are Pauli matrices and ∂_j spatial differential operators) obeys the relation

$$\sigma_1 H^T \sigma_1 = -H, \quad (4)$$

which constitutes class D according to Ref. [12]. The relation enables us to introduce the structure

$$\hat{G}(i\epsilon) = \begin{pmatrix} (H + i\epsilon)^{-1} & 0 \\ 0 & (H^T + i\epsilon)^{-1} \end{pmatrix} \quad (5)$$

for the dynamic description. This choice has a very important advantage over (3), since the upper

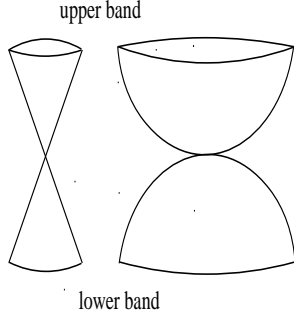


FIG. 1: Typical structure of two symmetric bands with a node with linear (left) and quadratic (right) dispersion.

and the lower block have the same determinant. Then the upper block can act on bosons and the lower block on fermions, providing us with a Bose-Fermi field theory and a nonlinear sigma model that has only a free massless Fermi (Grassmann) field [11, 13]. The latter describes diffusion and gives directly the experimentally observed minimal conductivity of graphene. Moreover, it reproduces the phase diagram (one metallic phase and two insulating Hall phases) of Refs. [14–17] for a nonzero average mass [13].

The disadvantage of (5) over the definition (3) is its restriction to the Dirac point, since a shift by a chemical potential $H \rightarrow H + \mu\sigma_0$ violates the relation (4). In the following we will start from (5) and extend it in such a way that a chemical potential can be included. This will give us a new dynamic structure with a continuous symmetry in Bose-Fermi space. The latter can be spontaneously broken and produce a two-component massless Fermi (Grassmann) field.

We consider a Hamiltonian with two bands whose dispersion is symmetric: $\pm E(\mathbf{k})$ with the 2D wavevector \mathbf{k} . Moreover, we assume particle-hole symmetry for the Hamiltonian

$$OH^TO = -H, \quad (6)$$

and include a node in the band structure (see Fig. 1). The node is important to create spontaneous symmetry breaking. This has been observed for gapped Dirac fermions, where the symmetry-breaking solution vanishes when the gap is too large [13].

In analogy to the Green's function in Eq. (5) we introduce $\hat{G}(i\epsilon) = (\hat{H} + i\epsilon)^{-1}$ with the extended

Hamiltonian

$$\hat{H} = \begin{pmatrix} H_+ & 0 & 0 & 0 \\ 0 & H_- & 0 & 0 \\ 0 & 0 & H_-^T & 0 \\ 0 & 0 & 0 & H_+^T \end{pmatrix} \quad H_{\pm} = H \pm \mu\sigma_0. \quad (7)$$

Then the matrix

$$\hat{S} = \begin{pmatrix} 0 & 0 & \varphi_1 O & 0 \\ 0 & 0 & 0 & \varphi_2 O \\ \varphi'_1 O & 0 & 0 & 0 \\ 0 & \varphi'_2 O & 0 & 0 \end{pmatrix} \quad (8)$$

with scalar variables φ_j, φ'_j anticommutes with \hat{H} : $\hat{S}\hat{H} = -\hat{H}\hat{S}$. This relation implies

$$e^{\hat{S}}\hat{H}e^{\hat{S}} = \hat{H} \quad (9)$$

which is a symmetry relation for the extended Hamiltonian with respect to $\hat{U} = e^{\hat{S}}$.

Now we use the matrix structure and apply it to a supersymmetric space that consists of four bosonic (upper) components and four fermionic (lower) components. In this representation we have to introduce the graded determinant det_g and the graded trace Tr_g (cf. [13]). For constructing the functional integral of the transition matrix K in Eq. (2) it is crucial that $\text{det}_g(\hat{H} + i\epsilon) = 1$ and $\text{det}_g(e^{\hat{S}}) = \exp(\text{Tr}_g \hat{S}) = 1$. Moreover, the variables φ_j in (8) are elements of a Grassmann algebra. Therefore, the symmetry is a supersymmetry, connecting bosonic with fermionic degrees of freedom. This symmetry is broken by the ϵ term though because \hat{U}^2 is not a unit matrix. Eqs. (7), (8) and (9) are the main results of this work. What remains to be discussed is the effect of the symmetry property on the transport for $\epsilon \rightarrow 0$, which will be studied by the standard nonlinear sigma model approach [8, 9, 19].

Nonlinear sigma model: The symmetry (9) is valid for any random H or μ , provided that H obeys (6). In order to calculate K it is necessary to specify the details of the randomness though. In the following we will consider a random gap because this has a strong effect due to backscattering (unlike a random μ , where backscattering is suppressed). For this purpose we consider an uncorrelated Gaussian distributed random gap with mean zero and variance g .

K in Eq. (2) can be expressed as a functional integral for a random term $v_{\mathbf{r}}\sigma_a$ in the Hamiltonian H [13] (a random gap is $a = 3$) with the action

$$S = \frac{1}{g} \text{Tr}_g(\hat{Q}^2) + \log \text{det}_g(\hat{H}_0 + i\epsilon\hat{\tau}_0 + \hat{\tau}_3\hat{Q}). \quad (10)$$

$\hat{Q}_{\mathbf{r}}$ is an 8×8 matrix field whose elements live on a superspace (the 4×4 diagonal blocks are

bosonic, the 4×4 off-diagonal blocks are fermionic) [11, 13]. We have used for the 8×8 matrix structure, where the hat $\hat{\cdot}$ means the generalization of a 2×2 to an 8×8 matrix structure (e.g. $\hat{\tau}_j = \text{diag}(\sigma_j, \sigma_j, \sigma_j, \sigma_j)$), in analogy to Eq. (7). The average Hamiltonian is $\hat{H}_0 = \langle \hat{H} \rangle$.

Without repeating here the derivation of the functional integral (cf. [13]) we switch directly to the saddle-point approximation of the integral, which allows us to focus on the role of the symmetry in Eq. (9) with the saddle point $\hat{Q}_0 = i\eta\hat{\tau}_3$, where the shift of the chemical potential μ has been included in \hat{H}_0 as $\mu \rightarrow \bar{\mu}$. From (10) we obtain

$$S_0 = \log \det g(\hat{H}_0 + i\epsilon\hat{\tau}_0 + \hat{\tau}_3\hat{Q}_0) ,$$

since the first term in (10) vanishes due to $\text{Tr}g(\hat{Q}_0^2) = 0$. Due to (9) there is a saddle-point manifold, when the parameters φ_j are replaced by spatially dependent Grassmann fields $\varphi_{j\mathbf{r}}$, that reads

$$\hat{Q}_0 \rightarrow \hat{Q}_{\mathbf{r}} = i\eta\hat{U}_{\mathbf{r}}^{-1}\hat{\tau}_3\hat{U}_{\mathbf{r}} = i\eta\hat{\tau}_3\hat{U}_{\mathbf{r}}^2 . \quad (11)$$

This provides the saddle-point action

$$S' = \log \left[\det g \left(\hat{H}_0 + i\epsilon + i\eta e^{2\hat{S}} \right) \right] , \quad (12)$$

and the transition matrix K now reads

$$K_{\mathbf{r}\mathbf{r}'} = 4 \frac{\eta^2}{g^2} \int \varphi_{j\mathbf{r}} \varphi'_{j\mathbf{r}'} e^{-S'} \mathcal{D}[\hat{Q}] . \quad (13)$$

We can expand S' in powers of η . This is also an expansion in powers of $\hat{G}_0 = (\hat{H}_0 + i(\epsilon + \eta)\hat{\tau}_0)^{-1}$, where the latter can be approximated by a gradient operator. This expansion is convergent, at least on large scales, when the gradient operator is small in comparison to η [18]. Up to second order in η it reads $S' \approx S_0 + S''$ with

$$S'' = 4i\eta \text{Tr}g \left(\hat{G}_0 \hat{S}^2 \right) - 8\eta^2 \text{Tr}g \left[\left(\hat{G}_0 \hat{S} \right)^2 \right] - 8\eta^2 \text{Tr}g \left[\left(\hat{G}_0 \hat{S}^2 \right)^2 \right] \quad (14)$$

and gives the standard form of the nonlinear sigma model [19] for the off-diagonal parts of the last two terms, whereas the first term and the diagonal part of the second term contribute to the symmetry-breaking term that is proportional to ϵ . Then the action separates into the two components as $S'' = S''_1 + S''_2$ with

$$S''_j = \frac{4\eta}{g} \sum_{\mathbf{r}} [\varphi_{j\mathbf{r}}(\epsilon - D\partial^2)\varphi'_{j\mathbf{r}} + \alpha_j \Phi_{j\mathbf{r}} \partial^2 \Phi_{j\mathbf{r}}] \quad (15)$$

with the field $\Phi_{j\mathbf{r}} = \varphi_{j\mathbf{r}}\varphi'_{j\mathbf{r}}$, the Laplacian $\partial^2 = \partial_1^2 + \partial_2^2$ and the Green's function $g_{\pm} = [H_0 + i(\epsilon + \eta) \pm \bar{\mu}]^{-1}$. The parameters for $\epsilon \sim 0$ read

$$\alpha = -\frac{\eta^2}{2} \text{Tr}_2(g_{+,0}^2 - g_{-,0}^2) = -i\eta^2 \text{Im} \text{Tr}_2(g_{+,0}^2) , \quad (16)$$

$\alpha_j = -(-1)^j \alpha$ and

$$D = -\frac{g\eta}{2} \frac{\partial^2}{\partial q_l^2} \int_{\mathbf{k}} \text{Tr}_2[g_{+, \mathbf{k}+\mathbf{q}/2}(i\eta)g_{+, \mathbf{k}-\mathbf{q}/2}(-i\eta)] \Big|_{\mathbf{q}=0} . \quad (17)$$

Thus our model depends only on the parameters g (disorder strength), η (scattering rate), and the renormalized chemical potential $\bar{\mu}$. For given g and μ the renormalized parameters η and $\bar{\mu}$ are determined as a solution of the saddle-point equation. Interestingly, α vanishes for $\bar{\mu} = 0$ such that the interaction disappears at the node (cf. [11]). Away from the node the interaction term in Eq. (15) can be treated in perturbation theory, where the perturbations are “dimers” on the lattice which cannot be visited by the random walk (diffusive path). This restricts the random walk but since the walk has no phase factor (it is a classical random walk since $(\epsilon - D\partial^2)^{-1}$ is a real symmetric matrix), there is no interference to generate Anderson localization.

According to (7) and (8), different values of j refer to different Fermi energies: $(H + i\epsilon + \mu)^{-1}$ (for $j = 1$) and $(H + i\epsilon - \mu)^{-1}$ (for $j = 2$). The different signs in front of α in Eq. (15) reflects the fact that α is proportional to μ . In the following we ignore the index j because its value affects only the sign of the coupling constant.

Random diffusion coefficient: Introducing the random variables $u_{\mathbf{r},k}$ with zero mean and variance 1, we can express the interaction term in (15) by the identity

$$\exp[\alpha(\partial_k \Phi_{\mathbf{r}})^2] = \langle \exp[i\sqrt{\alpha}(\partial_k \varphi_{\mathbf{r}})u_{\mathbf{r},k}(\partial_k \varphi'_{\mathbf{r}})] \rangle_u . \quad (18)$$

which allows us to rewrite K in (13). After having performed the φ integration we get

$$K_{\mathbf{r}\mathbf{r}'} = \frac{\eta}{g} \sum_{j=1,2} \langle \langle (\epsilon - D\partial^2 - i\sqrt{\alpha_j}u \cdot \partial^2)_{\mathbf{r}\mathbf{r}'}^{-1} \rangle \rangle_u , \quad (19)$$

where the average is with respect to the new distribution

$$\langle \langle \dots \rangle \rangle_u = \langle \dots \prod_{j=1,2} \det(\epsilon - D\partial^2 - i\sqrt{\alpha_j}u \cdot \partial^2) \rangle_u ,$$

i.e., the determinant is included in the distribution. In the representation (19) we have to average the diffusion propagator $(\epsilon - D\partial^2 - i\sqrt{\alpha_j}u \cdot \partial^2)^{-1}$ with a random diffusion coefficient. This can be done in

perturbation theory by expanding the propagator in powers of $\sqrt{\alpha}$, since α is small in the vicinity of the node. An alternative approach is a self-consistent Born approximation that formally takes into account a resummation of leading terms [20]. It is a saddle-point approximation for the integral over the random variables $u_{\mathbf{r},k}$ in Eq. (19). This approximation should be reliable, since there is no continuous degeneracy of saddle points as in the supersymmetric functional integral of Eq. (13). The saddle-point value \bar{u} implies for the diffusion coefficients $\bar{D}_j = D + i\sqrt{\alpha_j}\bar{u}$.

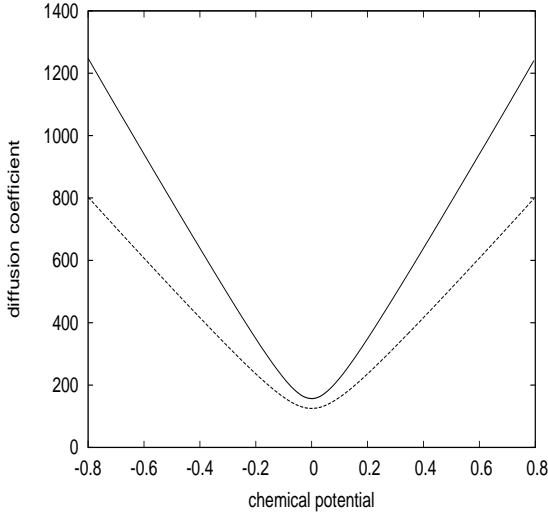


FIG. 2: Diffusion coefficient for 2D Dirac fermions (in arbitrary units) as a function of the renormalized chemical potential $\bar{\mu}$ for the scattering rate $\eta = 0.08$ (full curve) and $\eta = 0.1$ (dashed curve).

For a Dirac Hamiltonian $\langle H \rangle = i\sigma_k \partial_k$ (valid for a single node in graphene or for the surface of a topological insulator) we get $\bar{D}_j = D + (-1)^j D'$ with

$$D' \sim \alpha \lambda^2 / 4\pi D, \quad \alpha \sim -i \frac{\bar{\mu}}{\eta(1 + \eta^2/\lambda^2)},$$

where λ is the momentum cut-off. The Fourier components of $P_{\mathbf{r}} \equiv P_{\mathbf{r}0}$ in Eq. (1) then read

$$\tilde{P}_{\mathbf{q}} = \tilde{K}_{\mathbf{q}} / \tilde{K}_0 = \frac{\epsilon(\epsilon + Dq^2)}{(\epsilon + Dq^2)^2 + D'^2 q^4} \quad (20)$$

and the extension of the wavefunction $\sum_{\mathbf{r}} r_k^2 P_{\mathbf{r}}$

$$- \tilde{K}_{\mathbf{q}=0}'' / \tilde{K}_{\mathbf{q}=0} = 2D/\epsilon, \quad (21)$$

i.e., the correction D' drops out and only the diffusion coefficient D enters the final result. D is plotted in Fig. 2.

Although the dynamic conductivity is quite complex for Dirac particles [21], the DC conductivity can be extracted from the Einstein relation as

$$\sigma_{kk} \propto \rho D \frac{e^2}{h} \quad (22)$$

with the density of states at the Fermi level ρ . Since $D \sim D_0 |\bar{\mu}|$ (cf. Fig. 2) and $\rho \sim \rho_0 |\bar{\mu}|$ sufficiently far away from the node $\bar{\mu} = 0$ [3, 4], the conductivity increases with $|\bar{\mu}|^2$. This, on the other hand, is proportional to the quasiparticle density n . Consequently, the conductivity increases linearly with n and follows the same graphs as shown in Fig. 2, when the chemical potential is replaced by the quasiparticle density. These graphs are in agreement with the experimental observation [1, 2, 22].

In conclusion, we have found that the transport properties of a 2D electron gas with a spectral node are controlled by a dynamic symmetry. Spontaneous breaking of the symmetry generates a massless Fermi mode that leads to diffusion. For the special case of Dirac fermions this approach reproduces the well-known V shape of the conductivity.

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[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V. Dubonos, A.A. Firsov, *Nature* **438**, 197 (2005).
[2] Y. Zhang, Y.-W. Tan, H.L. Stormer, P. Kim, *Nature* **438**, 201 (2005).
[3] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, and A.K. Geim, *Rev. Mod. Phys.* **81**, 109 (2009).
[4] D.S.L. Abergel, V. Apalkov, J. Berashevich, K. Ziegler and T. Chakraborty, *Adv. Phys.* **59**, 261 (2010).

[5] X.-L. Qi and S.-C. Zhang, *Rev. Mod. Phys.* **83**, 1057 (2011).
[6] E. Abrahams, P.W. Anderson, D.C. Licciardello and T.V. Ramakrishnan, *Phys. Rev. Lett.* **42**, 673 (1979).
[7] E.N. Economou and M.H. Cohen, *Phys. Rev. Lett.* **25** (1970).
[8] L. Schäfer and F. Wegner, *Z. Physik B* **38**, 113 (1980).
[9] K. Efetov, *Supersymmetry in Disorder and Chaos* (Cambridge University Press 1997).

- [10] M. Bocquet, D. Serban and M.R. Zirnbauer, Nucl. Phys. B **578**, 628 (2000).
- [11] K. Ziegler, Phys. Rev. B **55**, 10661 (1997); Phys. Rev. Lett. **80**, 3113 (1998).
- [12] M.R. Zirnbauer, J. Math. Phys. **37**, 4986 (1996); A. Altland and M.R. Zirnbauer, Phys. Rev. B **55**, 1142 (1997).
- [13] K. Ziegler, Phys. Rev. Lett. **102**, 126802 (2009); Phys. Rev. B **79**, 195424 (2009).
- [14] T. Senthil and M.P.A. Fisher, Phys. Rev. B **61**, 9690 (2000).
- [15] J.T. Chalker, N. Read, V. Kagalovsky, B. Horovitz, Y. Avishai, A.W.W. Ludwig, Phys. Rev. B **65** 012506 (2001).
- [16] F. Evers and A.D. Mirlin, Rev. Mod. Phys. **80**, 1355 (2008).
- [17] M.V. Medvedyeva, J. Tworzydło, and C.W.J. Beenakker, Phys. Rev. B **81**, 214203 (2010).
- [18] K. Ziegler, J. Phys. A (in press).
- [19] S. Coleman, *Aspects of symmetry* (Cambridge University Press 1985).
- [20] N.H. Shon and T. Ando, J. Phys. Soc. Japan **67**, 2421 (1998).
- [21] M. Lewkowicz and B. Rosenstein, Phys. Rev. Lett. **102**, 106802 (2009).
- [22] J. H. Chen, C. Jang, M. S. Fuhrer, E. D. Williams, M. Ishigami, Nature Physics **4**, 377 (2008).